Quantum Transport on KAM Tori

Joachim Asch* Andreas Knauf†

November 1998

Abstract

Although quantum tunneling between phase space tori occurs, it is suppressed in the semiclassical limit $\hbar \searrow 0$ for the Schrödinger equation of a particle in $\mathbb{R}^d$ under the influence of a smooth periodic potential.

In particular this implies that the distribution of quantum group velocities near energy E converges to the distribution of the classical asymptotic velocities near E, up to a term of the order $\mathcal{O}(1/\sqrt{E})$.

1 Introduction

Consider abstractly a self-adjoint operator H on its domain $D(H)$ in a Hilbert space $\mathcal{H}$. Then for $\varepsilon \geq 0$ one may call a pair

$$(\tilde{\psi}, \tilde{E}) \in D(H) \times \mathbb{R} \quad , \quad \|\tilde{\psi}\| = 1 \quad , \quad \|(H - \tilde{E})\tilde{\psi}\| \leq \varepsilon$$

an ε-*quasimode* [1]. In particular, eigenfunctions ψ with eigenvalues E are 0-quasimodes.

The existence of an ε-quasimode $(\tilde{\psi}, \tilde{E})$ implies that the operator H has spectrum $\sigma(H)$ in $[\tilde{E} - \varepsilon, \tilde{E} + \varepsilon]$. In particular we are sure to find an eigenvalue E in an interval $[\tilde{E} - \mu, \tilde{E} + \mu]$ for $\varepsilon \leq \mu$, if we know that the spectrum in that interval is purely discrete.

*CPT-CNRS, Luminy Case 907, F-13288 Marseille Cedex 9, France. e-mail: asch@cpt.univ-mrs.fr

†Max-Planck-Institute for Mathematics in the Sciences, Inselstr. 22–26, D-04103 Leipzig, Germany. e-mail: knauf@mis.mpg.de

If we know in addition that E is the only such eigenvalue, then, after choosing an appropriate phase for its normalized eigenfunction ψ, we have

$$\|\tilde{\psi} - \psi\| \leq \frac{2\varepsilon}{\mu}. \tag{1}$$

However, due to near-degeneracies of $\sigma(H)$ there may be no eigenfunction of H near $\tilde{\psi}$:

The standard example is that of the Schrödinger operator on the line with the double well potential $V(q) := (q-1)^2(q+1)^2$. Then for energies $E < 1$ one may construct $\hbar^\infty$-quasimodes localized in one or the other well, whereas all eigenfunctions of $H^\hbar$ exhibit parity. Here the near-degeneracy of the eigenenergies, which is of order $\mathcal{O}(\exp(-c/\hbar))$, is connected with tunneling between the two components of the energy shell of the classical system (see, e.g. Lazutkin, [6]).

So in that case phase space tunneling survives the semiclassical limit, and one cannot confine a particle forever in a well. As a physical consequence one may mention the NH_3 microwave radiation.

For higher degrees of freedom d these energy shell components generalize to invariant Lagrangian tori in phase space. If such invariant tori exist and one has some control over the bicharacteristic flow in their vicinity, then it is possible to construct ε-quasimodes of high accuracy ($\varepsilon = \hbar^N$) and thus to extract precise spectral informations in the semiclassical limit $\hbar \searrow 0$, [6].

However, because of near-degeneracies in the spectrum, in general one cannot draw any conclusion concerning the semiclassical eigen*functions*.

In recent years refined epitactic methods allowed to produce semiconductors with periodic superlattices. The electrons in these periodic potentials have a small effective value of $\hbar$, leading to interesting effects (see [12]). In this context it is important to know to which extent one may model the electronic behavior classically.

This motivates our study of Schrödinger operators

$$H^\hbar = -\frac{\hbar^2}{2}\Delta + V \quad \text{on} \quad \mathcal{H} := L^2(\mathbb{R}^d)$$

whose potential $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$ is periodic w.r.t. a regular lattice $\mathcal{L} \subset \mathbb{R}^d$.

We may consider V as a function $V : \mathbb{T} \to \mathbb{R}$ on the d-torus $\mathbb{T} := \mathbb{R}^d/\mathcal{L}$.

The $\mathcal{L}$-invariance and the Bloch theorem imply that $H^\hbar$ conjugates unitarily to the direct integral of the operators

$$H^\hbar(k) := \tfrac{1}{2}(D+\hbar k)^2 + V \quad \text{on} \quad L^2(\mathbb{T}) \qquad (k \in \mathbb{T}^*), \tag{2}$$

acting on

$$\int_{\mathbb{T}^*}^{\oplus} L^2(\mathbb{T}, dq) \frac{dk}{\mathrm{vol}\mathbb{T}^*},$$

where $\mathcal{L}^*$ is the dual lattice with *Brillouin zone* $\mathbb{T}^* := \mathbb{R}^d/\mathcal{L}^*$ and $D := -i\hbar\nabla$ is the momentum operator. It follows that the spectrum consists of bands. Up to measure zero sets due to degeneracies, the eigenvalues $E_n^\hbar(k)$ are analytic in k, and are non-constant, (see, e.g.,Thomas [10], Wilcox [13], and Reed and Simon [9]). Thus the *group velocity* $\hbar^{-1}\nabla_k E_n^\hbar(k)$ vanishes at most on a set of measure zero.

On the other hand the symmetry $E_n^\hbar(-k) = E_n^\hbar(k)$ of the band functions implies in the non-degenerate case that the group velocity vanishes for $k=0$ and the other $2^d - 1$ fixed points of $k \mapsto -k$ on $\mathbb{T}^*$.

To see how this vanishing of the group velocity is connected with phase space tunneling, we consider the simplest case of $d=1$ dimension (for $d=2$ see also [4]).

In that case the energy shell $\Sigma_E := H^{-1}(E) \subset \mathcal{P}$ of the Hamiltonian function

$$H(p,q) := \tfrac{1}{2}p^2 + V(q) \quad \text{on the phase space} \quad \mathcal{P} := T^*\mathbb{T},$$

consists for energies $E > V_{\max} := \max_q V(q)$ of two components, corresponding to ballistic motion to the right resp. to the left. These components are permuted by the time reversal transformation $(p,q) \mapsto (-p,q)$ on $\mathcal{P}$.

As the eigenfunction $\psi_n^\hbar(k)$ can be chosen to be real for $k=0$, it is semiclassically equally concentrated on both (one-dimensional) tori corresponding to the energy $E = E_n^\hbar(0)$.

The vanishing group velocity is one manifestation of that fact. Thus for $k=0$, arbitrarily small values of $\hbar$ and large times t the quantum evolution $\exp(-iH^\hbar(k)t/\hbar)$ and the classical flow $\Phi^t : \mathcal{P} \to \mathcal{P}$ generated by H behave very differently.

However we argue that for general quasimomenta k in $\mathbb{T}^*$ *phase space tunneling is exceptional in the limit* $\hbar \searrow 0$.

More specifically, we conjectured in [2] that the quantum distribution of group velocities converges in the semiclassical limit to the classical one, see Conjecture 5.1 below.

We proved this in [2] for the extreme cases of potentials leading to ergodic motion, and for separable potentials (which are the only known examples of periodic potentials leading to integrable motion).

Here we show a similar statement for arbitrary smooth potentials and large energies, where KAM tori are known to dominate the phase space volume.

After presenting the strategy in *Sect. 2*, we adapt in *Sect. 3* Lazutkin's results on KAM-quasimodes to the present situation of a family $H^\hbar(k)$ of differential operators. *Thm. 4.1* contains our main result. It states that for large energies E a proportion $1 - \mathcal{O}(1/\sqrt{E})$ of the eigenfunctions is semiclassically concentrated near a KAM torus.

This then leads to a corresponding statement (*Thm. 5.3*) for the semiclassical distribution of group velocities, in accordance with the above conjecture.

In a final section, we try to abstract our strategy. We argue that a mere *existence proof* for a full set of $\hbar^N$–quasimodes with localized asymptotic velocities could imply the conjectured classical limit of the distribution of group velocities.

Acknowledgments. We thank Ruedi Seiler and SFB 288, TU Berlin, for hospitality, for which J.A. also thanks MPI in Leipzig.

2 Heuristics

Before we turn to formal statements and proofs, we shortly describe the main ideas, starting with the following observation.

Two given quasimodes associated to different KAM tori give rise to different expectations of the sub-principal symbol $\hbar k \cdot D$ of the operator $H^\hbar(k)$ defined in (2). Thus they can be separated energetically by varying the quasimomentum k, and for typical k in the Brillouin zone $\mathbb{T}^*$ one should not have too many near-degeneracies of energies.

Of course we must consider scales in order to make this argument work. In d dimensions the mean spacing $E^\hbar_{n+1}(k) - E^\hbar_n(k)$ between the eigenvalues of $H^\hbar(k)$ near $E > V_{\min}$ is of the order $\hbar^d$. Thus a priori one must consider in a fixed energy interval about $\hbar^{-d}$ quasimodes which may lead to a near-degeneracy with a given quasimode. For $\hbar^N$-quasimodes we need an energy separation of at least $\hbar^N$. So N should be larger than d.

Such high precision KAM quasimodes are constructed in the book [6] by Lazutkin (see also the article [11] by Thomas and Wassell for related results)

We apply this method after some straightforward adaptation to our family (2) of differential operators.

An important input for that construction consists in the refinement of KAM theory presented in the paper [7] by Pöschel. Roughly speaking one uses that the deviation of the Hamiltonian function H from an integrable one vanishes faster than any power of the phase space distance to the KAM set. In particular we may apply perturbative semiclassical techniques in some $\hbar^\alpha$-neighborhood of the set of KAM tori.

A final remark concerns the phase space complement of the KAM set. In general we do not have any information over individual eigenfunctions

and eigenvalues concentrating semiclassically in that region.

In particular we cannot hope to lift near-degeneracies between such eigenvalues and the energies of the KAM-quasimodes by changing the quasi-momentum. Moreover, if a quasimode is involved in such a near-degeneracy, there need not be any eigenfunction $\psi_n^\hbar(k)$ near to that quasimode.

However, we can apply a box counting principle. We know from KAM theory that for large energies E the complement of the KAM set is of relative measure $\mathcal{O}(1/\sqrt{E})$.

Then a Weyl argument implies that up to an exceptional set of relative size $\mathcal{O}(1/\sqrt{E})$ the eigenvalues $E_n^\hbar(k)$ near E are well-approximated by KAM quasimodes.

In the semiclassical limit these $\hbar^N$-quasimodes $(\tilde{\psi}, \tilde{E})$ are typically energetically separated in the sense that the associated intervals $[\tilde{E} - \hbar^N, \tilde{E} + \hbar^N]$ are disjoint. We have at least one eigenvalue $E_n^\hbar(k)$ in each such interval. Thus only an exceptional set of relative proportion $\mathcal{O}(1/\sqrt{E})$ of these intervals may contain more than one eigenvalue.

So for typical $k \in \mathbb{T}^*$ most $E_n^\hbar(k)$ are not near-degenerate, and thus the corresponding eigenfunctions $\psi_n^\hbar(k)$ are well approximated by quasimodes $\tilde{\psi}$.

3 KAM Estimates and Quasimodes

In order to apply KAM theory to H with energies in

$$I := [(1-\delta)E, (1+\delta)E] \tag{3}$$

near $E > 0$, we change coordinates. So consider the $d \times d$ matrix $L := (\ell_1, \ldots, \ell_d)/(2\pi)$ of a basis $(\ell_1, \ldots, \ell_d)$ for the configuration space lattice $\mathcal{L}$,

set $\hat{V}(\varphi) := V(L\varphi)$, denote by $\hat{\mathcal{P}} := T^*\hat{\mathbb{T}}$ the phase space over the standard torus

$$\hat{\mathbb{T}} := \mathbb{R}^d/(2\pi\mathbb{Z})^d$$

and define, using the matrix $M := (L^tL)^{-1}$, the Hamiltonian

$$\hat{H}_\varepsilon : \hat{\mathcal{P}} \to \mathbb{R} \quad , \quad \hat{H}_\varepsilon(J,\varphi) := \tfrac{1}{2}(J, MJ) + \varepsilon\hat{V}(\varphi).$$

Then for the diffeomorphism

$$\mathcal{M}_E : \mathcal{P} \to \hat{\mathcal{P}} \quad , \quad (p,q) \mapsto (J,\varphi) := \left(L^t p/\sqrt{E}, L^{-1}q\right)$$

we have

$$E \cdot \hat{H}_{1/E} \circ \mathcal{M}_E = H,$$

and the flow $\hat{\Phi}^t_\varepsilon$ generated by $\hat{H}_\varepsilon$ (w.r.t. the standard symplectic structure on $\hat{\mathcal{P}}$) is conjugate to the original flow, up to a change of time scale:

$$\hat{\Phi}^{\sqrt{E}t}_{1/E} \circ \mathcal{M}_E = \mathcal{M}_E \circ \Phi^t \qquad (t \in \mathbb{R}).$$

$\hat{\Phi}^t_\varepsilon$ becomes fully integrable for perturbation parameter $\varepsilon = 0$. Namely

$$\hat{\Phi}^t_0(J_0,\varphi_0) = (J_0, \varphi_0 + \omega_0(J_0)t)$$

with the *frequency vector*

$$\omega_0(J) := \frac{\partial \hat{H}_0}{\partial J}. \tag{4}$$

ω_0 is of independent variation, i.e. the matrix

$$\frac{\partial \omega_0(J)}{\partial J} = M \quad \text{is of rank} \quad d.$$

So we are in a situation to apply KAM theory, see [7]. For $\gamma > 0$ and $\tau > d-1$ we consider the Diophantine sets

$$\Omega_\gamma := \left\{\omega \in \mathbb{R}^d \mid \forall k \in \mathbb{Z}^d \setminus \{0\} : |\omega \cdot k| \geq \gamma \|k\|^{-\tau}\right\}. \tag{5}$$

These are asymptotically of full measure as $\gamma \searrow 0$.

Denote the interval of new energies by $\hat{I} := [1-\delta, 1+\delta]$. For $\varepsilon = 0$ the phase space region $\hat{\mathcal{P}}_\varepsilon := \hat{H}_\varepsilon^{-1}(\hat{I}) \subset \hat{\mathcal{P}}$ is of the form

$$\hat{\mathcal{P}}_0 = \hat{\mathcal{J}}^\infty \times \hat{\mathbb{T}}.$$

By KAM for $|\varepsilon|$ small there exist a smooth generating function $\hat{S}_\varepsilon$ on $\hat{\mathcal{J}}^\infty \times \hat{\mathbb{T}}$ and a Hamiltonian $\hat{K}_\varepsilon$ independent of the angle variables, with the following properties.

- The frequency vector

  $$\omega_\varepsilon : \hat{\mathcal{J}}^\infty \to \mathbb{R}^d \quad , \quad J^\infty \mapsto \nabla \hat{K}_\varepsilon(J^\infty)$$

  is nondegenerate, and coincides for $\varepsilon = 0$ with (4).

- On the Cantor set $\hat{\mathcal{J}}^\infty_{\gamma,\varepsilon} := (\omega_\varepsilon)^{-1}(\Omega_\gamma)$ of actions

  $$\hat{H}_\varepsilon(J^\infty - \partial_\varphi \hat{S}_\varepsilon(J^\infty, \varphi), \varphi) = \hat{K}_\varepsilon(J^\infty) \qquad \Big((J^\infty, \varphi) \in \hat{\mathcal{J}}^\infty_{\gamma,\varepsilon} \times \hat{\mathbb{T}}\Big).$$

- The symplectomorphism

  $$\hat{T}_\varepsilon : \hat{\mathcal{J}}^\infty \times \hat{\mathbb{T}} \to \hat{\mathcal{P}} \quad , \quad (J^\infty, \varphi^\infty) \mapsto (J, \varphi)$$

  generated by $J^\infty \varphi - \hat{S}_\varepsilon(J^\infty, \varphi)$ is near to the identity.

- For $\gamma = c\sqrt{\varepsilon}$ the set $\hat{\mathcal{K}}_\varepsilon := \hat{T}_\varepsilon(\hat{\mathcal{J}}^\infty_{\gamma,\varepsilon} \times \hat{\mathbb{T}}) \cap \hat{\mathcal{P}}_\varepsilon$ of $\hat{\Phi}^t$-invariant KAM tori is of Liouville measure

  $$\mathrm{vol}(\hat{\mathcal{K}}_\varepsilon) \geq \mathrm{vol}(\hat{\mathcal{P}}_\varepsilon) \cdot \big(1 - \mathcal{O}(\sqrt{\varepsilon})\big).$$

- The difference between the non-integrable Hamiltonian function $\hat{H}_\varepsilon(x)$ and the integrable Hamiltonian $\hat{K}_\varepsilon \circ \hat{T}_\varepsilon^{-1}(x)$ vanishes faster than any power of the distance $\mathrm{dist}(x, \hat{\mathcal{K}}_\varepsilon)$ from the invariant tori, and the same is true for any derivatives.

These statements imply corresponding results about the symplectic map T for the generating function $S := \sqrt{E}\hat{S}_{1/E} \circ \mathcal{M}_E$ and the integrable Hamiltonian $K := E \cdot \hat{K}_{1/E} \circ \mathcal{M}_E$

$$\mathcal{J}^{\infty}_{\gamma,E} := \sqrt{E}(L^t)^{-1}\hat{\mathcal{J}}^{\infty}_{\gamma,1/E}$$

and the subset

$$\mathcal{K}_I := \mathcal{M}_E^{-1}(\hat{\mathcal{K}}_\varepsilon) \subset \mathcal{P}_I := H_0^{-1}(I). \tag{6}$$

of KAM tori for the flow Φ^t. In particular,

$$\mathrm{vol}(\mathcal{K}_I) \geq \mathrm{vol}(\mathcal{P}_I) \cdot \left(1 - \mathcal{O}(E^{-1/2})\right). \tag{7}$$

Turning to quantum mechanics, the following theorem was essentially proven by Lazutkin in [6].

Theorem 3.1 *Let $\tau > 2d$ in (5), $0 < \hbar < 1$ and $k \in \mathbb{T}^*$. Define for $\alpha \in (1, \frac{\tau-d}{d})$*

$$\Lambda^\hbar_I(k) := \{\ell^* \in \mathcal{L}^* \mid \mathrm{dist}(\hbar(\ell^* + k), \mathcal{J}^{\infty}_{\gamma,E}) \leq \hbar^\alpha\}.$$

Then for $\beta := 1 - \alpha d/(\tau - d) > 0$

1. $$(2\pi\hbar)^d |\Lambda^\hbar_I(k)| = |\mathcal{K}_I| + \mathcal{O}\left(\hbar^\beta\right). \tag{8}$$

Furthermore for $N \in \mathbb{N}$, $\hbar$ small enough and $\ell^* \in \Lambda^\hbar_I(k)$ there exists a $\hbar^{N+1}$–quasimode $(\tilde{E}^\hbar_{\ell^*}(k), \tilde{\psi}^\hbar_{\ell^*}(k))$. It follows that:

2. *there is an eigenvalue $E^\hbar(k)$ of $H^\hbar(k)$ with*
$$|E^\hbar(k) - \tilde{E}^\hbar_{\ell^*}(k)| \leq \hbar^{N+1};$$

3. *for the spectral projection P on $(E^\hbar(k) - \hbar^p, E^\hbar(k) + \hbar^p)$ it holds*
$$\|(\hat{\mathbb{1}} - P)\tilde{\psi}^\hbar_{\ell^*}(k)\| \leq \hbar^{N+1-p}.$$

4. *Let $N > 2d + 2$ and $0 < p < N + 1 - d$. Then $\forall \varepsilon > 0\ \exists \alpha$ such that the dimension $\mathbf{N}$ of the space of all these quasimodes projected to the spectral subspace of $\bigcup_{\ell^*}(E^\hbar(k) - \hbar^p, E^\hbar(k) + \hbar^p)$ meets the estimate*
$$(2\pi\hbar)^d \mathbf{N} = |\mathcal{K}_I| + \mathcal{O}\left(\hbar^{1-\varepsilon}\right). \tag{9}$$

Proof. This is essentially Theorem 41.10 in [6]. We specialize some formal aspects to our case – i.e. the configuration manifold has no boundary and the invariant Lagrangian tori are diffeomorphically projecting to the configuration torus, so that we do not need a Maslov operator.
(ad 1): This is Lazutkin's Proposition 40.2.
(ad 2 and 3): Let E be so large, that the KAM results hold true. The Ansatz for the quasimodes is:

$$\tilde{E}^{\hbar}(k) = \sum_{j=0}^{N+1} \hbar^j E_j(k), \quad \tilde{\psi}^{\hbar}(k)(q) = e^{\frac{i}{\hbar}(S(k,q)-\hbar\langle k,q\rangle)} \sum_{j=0}^{N} \hbar^j A_j(k,q) \tag{10}$$

with

$$\begin{aligned} &A_j(k,.) \in C^\infty(\mathbb{T}) \quad , \\ &S(k,.) \in C^\infty(\mathbb{R}^d) \quad , \quad S(k,q+\ell) - S(k,q) - \hbar\langle k,\ell\rangle \in 2\pi\mathbb{Z} \quad (\ell \in \mathcal{L}). \end{aligned} \tag{11}$$

Employing the operators

$$T_k := -\frac{i}{2}(\partial_q S \partial_q + \partial_q \partial_q S) = -i((\nabla_q S)\cdot\nabla_q + \tfrac{1}{2}\Delta S)),$$

one computes

$$\begin{aligned} &e^{-\frac{i}{\hbar}(S-\hbar\langle k,q\rangle)} \left(H^{\hbar}(k) - \sum_{j=0}^{N+1} \hbar^j E_j \right) \tilde{\psi}^{\hbar}(k)(q) = \\ &\quad \left(\tfrac{1}{2}(\partial_q S)^2 + V - E_0\right) \sum_{j=0}^{N} \hbar^j A_j + \\ &\quad \sum_{j=0}^{N} \hbar^{j+1} T_k A_j - \tfrac{1}{2} \sum_{j=1}^{N+1} \hbar^{j+1} \Delta A_{j-1} - \sum_{j=0}^{2N} \hbar^{j+1} \sum_{l=\max(0,j-N)}^{\min(N,j)} E_{j+1-l} A_l \end{aligned} \tag{12}$$

and is led to consider the equations

$$H(\partial_q S(k,q),q) - E_0(k) = \mathcal{O}\left(\hbar^\infty\right) \tag{$(SC)_{-1}$}$$

and for $0 \le j \le N$, with $A_{-1} := 0$

$$T_k A_j(k) - \tfrac{1}{2}\Delta A_{j-1}(k) + \textstyle\sum_{l=0}^{j} E_{j+1-l}(k) A_l(k) = \mathcal{O}\left(\hbar^\infty\right) \tag{$(SC)_j$}$$

with the boundary conditions specified in (11).

The first step is to find a solution of the Hamilton-Jacobi equation $(SC)_{-1}$. By KAM we know that there exists $K \in C^\infty(\mathcal{J}^\infty), S \in C^\infty(\mathcal{J}^\infty \times \mathbb{T})$ such that not only

$$H(P - \partial_q S(P,q), q) = K(P) \quad \text{on } (\partial_P K)^{-1}(\Omega_\gamma) \times \mathbb{T}$$

but

$$H(P - \partial_q S(P,q), q) = K(P) + \mathcal{O}\left(\mathrm{dist}(P, (\partial_P K)^{-1}(\Omega_\gamma))^\infty\right) \tag{13}$$

on $\mathcal{J}^\infty \times \mathbb{T}$ with all derivatives. Now set

$$\begin{aligned} \tilde{S}(P,q) &:= Pq - S(P,q). \\ S(\ell^*, k, q) &:= \tilde{S}(\hbar(\ell^* + k), q), \quad E_0(\ell^*, k) := K(\hbar(k + \ell^*)) \end{aligned} \tag{14}$$

then defines a solution of $(SC)_{-1}$.

Using the same strategy the transport equations $(SC)_j$ are now solved in two steps: first solve the corresponding equation indexed by P approximatively near a KAM torus, then replace P by $\hbar(\ell^* + k)$ for $\ell^* \in \Lambda_I^\hbar(k)$ and exploit flatness of the functions.

Let E be so large that $\partial^2_{qP}\tilde{S}(P,q)$ is non-degenerate. $|\det \partial^2_{qP}\tilde{S}(P,q)|\, dq$ is (the coordinate representation of) an invariant measure on a KAM torus $P = const$. So, with T_P denoting the transport operator with respect to $\tilde{S}(P,q)$:

$$(\partial_q \tilde{S} \partial_q + (\Delta \tilde{S}))|\det \partial^2_{qP}\tilde{S}(P,q)| = 0 \Longleftrightarrow T_P \underbrace{\sqrt{|\det \partial^2_{qP}\tilde{S}(P,q)|}}_{=:A_0(P,q)} = 0.$$

For arbitrary P it follows that $T_P A_0(P,q) = \mathcal{O}\left(\mathrm{dist}(P, (\partial_P K)^{-1}(\Omega_\gamma))^\infty\right)$ so

$$A_0(q, \ell^*, k) := A_0(q, \hbar(\ell^* + k)), \qquad E_1 := 0 \tag{15}$$

satisfy $(SC)_0$ for $\ell^* \in \Lambda_I^\hbar(k)$.

By (15) we may now suppose that $A_0(P,q), E_1(P) \ldots A_j(P,q), E_{j+1}(P)$ meet

$$(T_P A_{j'} - \tfrac{1}{2}\Delta A_{j'-1} + \textstyle\sum_{l=0}^{j'-1} E_{j'+1-l} A_l)(P,q) = \mathcal{O}\left(\mathrm{dist}(P, (\partial_P K)^{-1}(\Omega_\gamma))^\infty\right).$$

Then the structure of the equation for A_{j+1}, E_{j+2} is

$$T_P A_{j+1}(P,q) = f(P,q) + E_{j+2}(P) A_0(P,q). \tag{16}$$

This is satisfied for $P \in (\partial_P K)^{-1}(\Omega_\gamma)$ by

$$E_{j+2}(P) := -\int_{\mathbb{T}} A_0^{-1} f(P, q(P,Q))\, dQ$$

$$A_{j+1}(P, q(P,Q)) := A_0(P, q(P,Q)) \sum_{0 \neq \ell^* \in \mathcal{L}^*} \frac{(A_0^{-1} f)\hat{}(\ell^*, P)}{\langle \partial_P K(P), \ell^* \rangle} e^{i\langle Q, \ell^* \rangle}.$$

Here $q(P,Q)$ is given by the canonical diffeomorphism $T : (P,Q) \mapsto (p,q)$ generated by $\tilde{S}(P,q)$, and $g \mapsto \hat{g}$ the Fourier-Transform

$$\hat{g}(\ell^*, P) := \int_{\mathbb{T}} g(P,Q) e^{-i\langle Q, \ell^* \rangle} dQ.$$

Indeed, equation (16) is equivalent to

$$\begin{aligned}
&(-i\partial_q \tilde{S} \partial_q (A_0^{-1} A_{j+1}) = A_0^{-1} f + E_{j+2})(P,q) \Longleftrightarrow \\
&-i\frac{d}{dt} A_0^{-1} A_{j+1} \circ \Phi^t(\partial_q \tilde{S}(P,q), q) \restriction_{t=0} = (A_0^{-1} f + E_{j+2})(P,q)
\end{aligned}$$

where Φ^t is the Hamiltonian flow of H. But $A_0^{-1} A_{j+1} \circ \Phi^t \circ T^{-1} = A_0^{-1} A_{j+1} \circ T^{-1} \circ \Psi^t$ where $\Psi^t(P,Q) = (P, Q + \partial_P K t)$ is the flow generated by K. So equation (16) is met by the above defined objects which are well defined and smooth if P labels a KAM torus and have a Whitney extension to $\mathcal{J}^\infty \times \mathbb{T}$. So by the same argument as before

$$A_{j+1}(\ell^*, k, q) := A_{j+1}(q, \hbar(\ell^* + k)), \quad E_{j+1}(\ell^*, k) := E_{j+1}(\hbar(\ell^* + k))$$

satisfy $(SC)_{j+1}$.

Define now with the functions so obtained the quasimode $(\tilde{\psi}^\hbar_{\ell^*}(k), \tilde{E}^\hbar_{\ell^*}(k))$ by the formula (10) with $\tilde{\psi}^\hbar_{\ell^*}(k)$ normalized and the sum running up to N; the sum for $\tilde{E}^\hbar_{\ell^*}(k)$ runs up to $N+1$. We then have

$$(H^\hbar(k) - \tilde{E}^\hbar_{\ell^*}(k))\tilde{\psi}^\hbar_{\ell^*}(k) = \mathcal{O}\left(\hbar^{N+2}\right)$$

so choosing $\hbar$ small enough we get the assertion. Items 2 and 3 follow by general considerations about quasimodes.

(ad 4): To deduce (9) one has to estimate $\langle \tilde{\psi}^\hbar_{\ell^*}(k), \tilde{\psi}^\hbar_{m^*}(k) \rangle$, which is Lazutkin's Proposition 41.9. $\square$

Remark 3.2 By [7] it suffices to assume that the potential $V \in C^l(\mathbb{T}, \mathbb{R})$ for $l \in \mathbb{N}$ large enough.

4 Approximation of Eigenfunctions

Let the $\hbar^{2N}$–quasimodes $\{(\tilde{\psi}^{\hbar}_{\ell^*}(k), \tilde{E}^{\hbar}_{\ell^*}(k))\}_{\ell^* \in \Lambda^{\hbar}_I(k)}$ be given by Thm. 3.1 and denote by

$$P^{\hbar}_{\ell^*}(k) \qquad (\ell^* \in \Lambda^{\hbar}_I(k))$$

the spectral projector for $H^{\hbar}(k)$ and the interval $[\tilde{E}^{\hbar}_{\ell^*}(k) - \hbar^N, \tilde{E}^{\hbar}_{\ell^*}(k) + \hbar^N]$. For each $\ell^* \in \Lambda^{\hbar}_I(k)$ there is a nearby eigenvalue

$$E^{\hbar}_n(k) \quad \text{with} \quad |E^{\hbar}_n(k) - \tilde{E}^{\hbar}_{\ell^*}(k)| \le \hbar^{2N}. \tag{17}$$

So for $\hbar < \hbar_0$ we know in particular that $\dim(P^{\hbar}_{\ell^*}(k)) \ge 1$.

But since the quasimode construction is only based on the KAM part of phase space, it does not suffice to know that the quasimode energies $\tilde{E}^{\hbar}_{\ell^*}(k)$ are separated from each other to ensure that the eigenenergies are isolated. Thus we consider the subset

$$\mathcal{F}\Lambda^{\hbar}_I(k) := \{\ell^* \in \mathcal{G}\Lambda^{\hbar}_I(k) \mid \dim(P^{\hbar}_{\ell^*}(k)) = 1\} \qquad (k \in \mathbb{T}^*). \tag{18}$$

of the index set

$$\mathcal{G}\Lambda^{\hbar}_I(k) := \left\{\ell^* \in \Lambda^{\hbar}_I(k) \mid |\tilde{E}^{\hbar}_{\ell^*}(k) - \tilde{E}^{\hbar}_{\ell'}(k)| > 2\hbar^N \text{ for } \ell' \in \Lambda^{\hbar}_I(k)\backslash_{\{\ell^*\}}\right\},$$

We obtain a map

$$\mathcal{I}_k : \mathcal{G}\Lambda^{\hbar}_I(k) \to \mathbb{N}$$

by setting $\mathcal{I}_k(\ell^*) := n$ for some n meeting (17). This map is one-to-one.

Its restriction to $\mathcal{F}\Lambda^{\hbar}_I(k)$ is uniquely defined, since for $\ell^* \in \mathcal{F}\Lambda^{\hbar}_I(k)$ $P^{\hbar}_{\ell^*}(k)$ is the one-dimensional projector for the eigenfunction $\psi^{\hbar}_{\mathcal{I}_k(\ell^*)}(k)$ of $H^{\hbar}(k)$ whose eigenvalue $E^{\hbar}_{\mathcal{I}_k(\ell^*)}(k)$ lies in $[\tilde{E}^{\hbar}_{\ell^*}(k) - \hbar^N, \tilde{E}^{\hbar}_{\ell^*}(k) + \hbar^N]$.

The index set $\mathcal{G}\Lambda^{\hbar}_I(k)$ of the separated quasimodes may be very small. For example it is even empty for $k = 0$ in $d = 1$ dimensions, if $\hbar > 0$ is small enough. However, its *mean* cardinality

$$\left\langle |\mathcal{G}\Lambda^{\hbar}_I| \right\rangle := \int_{\mathbb{T}^*} |\mathcal{G}\Lambda^{\hbar}_I(k)| \frac{dk}{\mathrm{vol}\mathbb{T}^*}$$

over the Brillouin zone turns out to be asymptotic to

$$\left\langle |\mathcal{G}\Lambda^{\hbar}_I| \right\rangle \sim (2\pi\hbar)^{-d} \mathrm{vol}(\mathcal{K}_I),$$

with the KAM subset $\mathcal{K}_I$ as defined in (6). This is the reason why indices in $\mathcal{F}\Lambda^{\hbar}_I(k)$ are abundant on the average; it holds:

Theorem 4.1 *For $\ell^* \in \mathcal{F}\Lambda_I^\hbar(k)$, $k \in \mathbb{T}^*$ and a suitable choice of phase of the eigenfunction $\psi^\hbar_{\mathcal{I}_k(\ell^*)}(k)$,*

$$\|\psi^\hbar_{\mathcal{I}_k(\ell^*)}(k) - \tilde{\psi}^\hbar_{\ell^*}(k)\| \le 2\hbar^N. \tag{19}$$

For $N > d+2$ there is a $\beta > 0$ such that for $I := [(1-\delta)E, (1+\delta)E]$ with $E > E_{\rm th}$

$$\mathrm{vol}(\mathcal{K}_I) - \mathrm{vol}(\mathcal{K}_I^c) - \mathcal{O}_E(\hbar^\beta) \le (2\pi\hbar)^d \left\langle |\mathcal{F}\Lambda_I^\hbar| \right\rangle \le \mathrm{vol}(\mathcal{K}_I) + \mathcal{O}_E(\hbar^\beta), \tag{20}$$

with $\mathcal{K}_I^c := \mathcal{P}_I \setminus \mathcal{K}_I$. In particular

$$\left| \frac{(2\pi\hbar)^d \left\langle |\mathcal{F}\Lambda_I^\hbar| \right\rangle}{\mathrm{vol}(\mathcal{P}_I)} - 1 \right| \le \sqrt{\frac{E_{\rm th}}{E}} + \mathcal{O}_E(\hbar^\beta). \tag{21}$$

Remark 4.2 The Liouville measure of the thickened energy shell is of order

$$\mathrm{vol}(\mathcal{P}_I) = c(\delta) \cdot E^{d/2} \cdot (1 + \mathcal{O}(1/E)). \tag{22}$$

Proof. Estimate (19) follows from (1) and Def. (18), since the $(\tilde{\psi}^\hbar_{\ell^*}(k), \tilde{E}^\hbar_{\ell^*}(k))$ are $\hbar^{2N}$-quasimodes.

The upper bound in (20) follows from the Lazutkin result (8) for $|\Lambda_I^\hbar(k)|$.

We claim that

$$(2\pi\hbar)^d \left\langle |\mathcal{G}\Lambda_I^\hbar| \right\rangle \ge \mathrm{vol}(\mathcal{K}_I) - \mathcal{O}(\hbar^\beta). \tag{23}$$

By (8) this follows from an estimate of the form

$$(2\pi\hbar)^d \left\langle |\Lambda_I^\hbar \setminus \mathcal{G}\Lambda_I^\hbar| \right\rangle = \mathcal{O}(\hbar^\beta). \tag{24}$$

But

$$\left\langle |\Lambda_I^\hbar \setminus \mathcal{G}\Lambda_I^\hbar| \right\rangle \le \int_{\mathbb{T}^*} \sum_{\ell_1 \ne \ell_2 \in \Lambda_I^\hbar} \chi\left(\tilde{E}^\hbar_{\ell_1}(k) - \tilde{E}^\hbar_{\ell_2}(k) \right) \frac{dk}{\mathrm{vol}\mathbb{T}^*}, \tag{25}$$

where $\chi(x) := 1$ for $|x| \le 2\hbar^N$ and 0 otherwise.

For E large and $\hbar < \hbar_0$

$$\begin{aligned} \left| \nabla \left(\tilde{E}^\hbar_{\ell_1}(k) - \tilde{E}^\hbar_{\ell_2}(k) \right) \right| &\ge \tfrac{1}{2} \left| \nabla \left(E_0(\ell_1, k) - E_0(\ell_2, k) \right) \right| \\ &\ge \tfrac{1}{4} \hbar^2 |\ell_1 - \ell_2| \ge cte.\hbar^2 \end{aligned}$$

uniformly for all $k \in \mathbb{T}^*$ and $\ell_1 \neq \ell_2 \in \Lambda_I^\hbar$. Thus by the implicit function theorem the set of quasimomenta $k \in \mathbb{T}^*$ leading to a degeneracy

$$\tilde{E}_{\ell_1}^\hbar(k) = \tilde{E}_{\ell_2}^\hbar(k)$$

of quasi-energies forms a hypersurface, and

$$\int_{\mathbb{T}^*} \chi\left(\tilde{E}_{\ell_1}^\hbar(k) - \tilde{E}_{\ell_2}^\hbar(k)\right) \frac{dk}{\mathrm{vol}\mathbb{T}^*} = \mathcal{O}(\hbar^{N-2}).$$

Since $|\Lambda_I^\hbar|$ is of order $\mathcal{O}(\hbar^{-d})$, the r.h.s. of (25) is thus of order $\mathcal{O}(\hbar^{-2d+N-2})$. So for $N > d+2+\beta$ estimate (24) holds true, implying (23).

We estimate the number

$$\left\langle |\mathcal{F}\Lambda_I^\hbar| \right\rangle = \left\langle |\mathcal{G}\Lambda_I^\hbar| \right\rangle - \left\langle |\mathcal{G}\Lambda_I^\hbar \setminus \mathcal{F}\Lambda_I^\hbar| \right\rangle \tag{26}$$

from below by using (23) and the relation

$$\left|\mathcal{G}\Lambda_I^\hbar(k) \setminus \mathcal{F}\Lambda_I^\hbar(k)\right| \leq \left|\Xi_I^\hbar(k) \setminus \mathcal{I}_k(\mathcal{G}\Lambda_I^\hbar(k))\right|, \qquad (k \in \mathbb{T}^*) \tag{27}$$

where

$$\Xi_I^\hbar(k) := \{n \in \mathbb{N} \mid E_n^\hbar(k) \in I\}$$

is the index set of all eigenvalues in the interval I.

Estimate (27) follows by noting that its l.h.s. equals the number of intervals

$$[\tilde{E}_{\ell^*}^\hbar(k) - \hbar^N, \tilde{E}_{\ell^*}^\hbar(k) + \hbar^N] \quad \text{for} \quad \ell \in \mathcal{G}\Lambda_I^\hbar(k)$$

containing two or more eigenvalues $E_n^\hbar(k)$ (counted with multiplicity). By definition of $\mathcal{G}\Lambda_I^\hbar(k)$ these intervals are disjoint, and we have

$$E_{\mathcal{I}_k(\ell^*)}^\hbar(k) \in [\tilde{E}_{\ell^*}^\hbar(k) - \hbar^N, \tilde{E}_{\ell^*}^\hbar(k) + \hbar^N],$$

so that further eigenvalues must be indexed by an integer belonging to the set which appears on the r.h.s. of (27).

The Weyl estimate

$$(2\pi\hbar)^d \left|\Xi_I^\hbar(k)\right| = \mathrm{vol}(\mathcal{P}_I) + \mathcal{O}(\hbar) \qquad (k \in \mathbb{T}^*)$$

is uniform in k, since the slope of the band functions is bounded above by

$$|\nabla_k E_n^\hbar(k)| \leq \hbar\sqrt{2(E_n^\hbar(k) - V_{\min})}$$

and thus of order $\hbar$ if $E_n^\hbar(k) \in I$ (see [2], Corr. 2.4).

Thus the r.h.s. of (27) is bounded above by

$$\left|\Xi_I^\hbar(k) \setminus \mathcal{I}_k(\mathcal{G}\Lambda_I^\hbar(k))\right| \leq (2\pi\hbar)^{-d}\mathrm{vol}(\mathcal{P}_I) - |\mathcal{G}\Lambda_I^\hbar(k)| - \mathcal{O}(\hbar^{1-d}).$$

Inserting that upper estimate for (27) in (26) and using (23) proves the lower bound in (20).

Finally, estimate (21) follows from (20) and the result

$$\frac{\mathrm{vol}(\mathcal{K}_I^c)}{\mathrm{vol}(\mathcal{P}_I)} = \mathcal{O}\left(1/\sqrt{E}\right),$$

see (7). □

5 Asymptotic Velocity

As a consequence of Birkhoff's Ergodic Theorem for λ–almost all $x_0 \in \mathcal{P}$

$$\bar{v}^\pm(x_0) := \lim_{T\to\pm\infty} \frac{1}{T}\int_0^T p(t, x_0)dt$$

exist and are equal (λ denoting the Liouville measure on $\mathcal{P}$). In this case we set $\bar{v}(x_0) := \bar{v}^\pm(x_0)$, and otherwise $\bar{v}(x_0) := 0$, thus defining the *asymptotic velocity*

$$\bar{v} : \mathcal{P} \to \mathbb{R}^d$$

which is a λ–measurable phase space function.

We are particularly interested in the energy dependence of asymptotic velocity and thus introduce the *energy-velocity map*

$$A := (H, \bar{v}) : \mathcal{P} \to \mathbb{R}^{d+1}. \tag{28}$$

A is λ–measurable and generates an image measure $\nu := \lambda A^{-1}$ on $\mathbb{R}^{d+1}$.

On the other hand (see [2]) for almost all $k \in \mathbb{T}^*$ the operator of asymptotic velocity

$$\bar{v}^\hbar(k) := \lim_{T\to\infty} \frac{1}{T}\int_0^T e^{iH^\hbar(k)t}(D + \hbar k)e^{-iH^\hbar(k)t}\; dt.$$

exists and is given by

$$\bar{v}^\hbar(k) = \sum P_m^\hbar(k)(D + \hbar k)P_m^\hbar(k) = \sum \hbar^{-1}\nabla_k E_m^\hbar(k) P_m^\hbar(k)$$

with the eigenprojections $P_m^\hbar(k)$ of $H^\hbar(k)$.

The *quantum asymptotic velocities* are defined by

$$\bar{v}_n^\hbar(k) := \begin{cases} \hbar^{-1}\nabla_k E_n^\hbar(k) & \text{, gradient exists} \\ 0 & \text{, otherwise.} \end{cases}$$

We equip the *semiclassical phase space* $\mathcal{P}^\hbar := \mathbb{N} \times \mathbb{T}^*$ with the *semiclassical measure* $\lambda^\hbar := (2\pi\hbar)^d \mu_1 \times \mu_2$, where μ_1 denotes counting measure on $\mathbb{N}$ and μ_2 Haar measure on the Brillouin zone $\mathbb{T}^*$.

In order to compare classical and quantum quantities, we introduce the *energy-velocity map*

$$A^\hbar : \mathcal{P}^\hbar \to \mathbb{R}^{d+1} \quad \text{with} \quad A^\hbar(n,k) := (E_n^\hbar(k), \bar{v}_n^\hbar(k))$$

and the image measure $\nu^\hbar := \lambda^\hbar (A^\hbar)^{-1}$.

Example: For $V \equiv 0$ (free motion) $\nu^\hbar = \nu$ independent of the value of $\hbar$.

In [2] we stated the following conjecture, which we proved for smooth V leading to integrable resp. to ergodic motion (see also [5] for ergodic motions generated by Coulombic periodic V):

Conjecture 5.1 *For all $\mathcal{L}$–periodic potentials $V \in C^\infty(\mathbb{R}^d, \mathbb{R})$*

$$w^* - \lim_{\hbar \searrow 0} \nu^\hbar = \nu$$

(which means $\lim_{\hbar\searrow 0} \int_{\mathbb{R}^{d+1}} f(x) d\nu^\hbar(x) = \int_{\mathbb{R}^{d+1}} f(x) d\nu(x)$ for continuous functions $f \in C_0^0(\mathbb{R}^{d+1}, \mathbb{R})$ of compact support).

Remark 5.2 One may also consider the stronger conjecture with continuous *bounded* test functions f, that is weak convergence in the language of probability theory.

Here we obtain a statement which verifies the conjecture in the high energy limit. To this aim we introduce the *ballistic scaling*

$$f_E(e,v) := E^{-d/2} f(e/E, v/\sqrt{E}) \qquad (E > 0)$$

of a test function $f \in C_0^0(\mathbb{R}^{d+1},\mathbb{R})$, so that $f_1 = f$. We notice that for $V \equiv 0$ we have $\nu(E,v) = C \cdot \delta(E - \frac{1}{2}v^2)$ so that

$$\int_{\mathbb{R}^{d+1}} f_E(x)d\nu(x) \equiv \int_{\mathbb{R}^{d+1}} f(x)d\nu(x) \qquad (E>0).$$

The result is

Theorem 5.3 *For all $f \in C^0(\mathbb{R}^{d+1},\mathbb{R})$ with compact support in $\mathbb{R}^+ \times \mathbb{R}^d$ we have*

$$\limsup_{\hbar\searrow 0} \left| \int_{\mathbb{R}^{d+1}} f_E(x)d\nu^\hbar(x) - \int_{\mathbb{R}^{d+1}} f_E(x)d\nu(x) \right| = \mathcal{O}(1/\sqrt{E}). \tag{29}$$

Proof. By our assumption on f there is an interval I of the form (3) so that $I \times \mathbb{R}^d$ strictly contains the support of f_E.

The index set of eigenenergies in I splits into the disjoint union

$$\Xi_I^\hbar(k) = \Xi_1^\hbar(k) \cup \Xi_2^\hbar(k) \quad \text{with} \quad \Xi_1^\hbar(k) := \mathcal{I}_k(\mathcal{F}\Lambda_I^\hbar(k)).$$

By (21), the volume estimate (22) and injectivity of $\mathcal{I}_k$

$$(2\pi\hbar)^d \left\langle |\Xi_2^\hbar| \right\rangle = \mathcal{O}(E^{(d-1)/2}) + \mathcal{O}_E(\hbar^\beta),$$

so that

$$(2\pi\hbar)^d \int \sum_{n\in\Xi_2^\hbar(k)} f_E(E_n^\hbar(k), \bar{v}_n^\hbar(k))dk = \mathcal{O}(1/\sqrt{E}) + \mathcal{O}_E(\hbar^\beta).$$

This leads to a contribution of order $\mathcal{O}(1/\sqrt{E})$ to (29), so that we need only estimate the contribution of $\Xi_1^\hbar$. By (8)

$$\lim_{\hbar\searrow 0}(2\pi\hbar)^d \left\langle |\Lambda_I^\hbar \setminus \Lambda_1^\hbar| \right\rangle = 0 \quad \text{for} \quad \Lambda_1^\hbar(k) := \{\ell^* \in \Lambda_I^\hbar(k) \mid \hbar(\ell^*+k) \in \mathcal{J}_{\gamma,E}^\infty\}.$$

So it suffices to consider the contribution of the index set

$$\Xi_{1,1}^\hbar(k) := \mathcal{I}_k(\mathcal{F}\Lambda_I^\hbar(k) \cap \Lambda_1^\hbar(k)) \subset \Xi_1^\hbar(k).$$

The result (29) then follows from the estimate

$$\bar{v}_n^\hbar(k) = \partial_P K(\hbar(\ell^*+k)) + \mathcal{O}(\hbar). \tag{30}$$

for $\ell^* \in \mathcal{F}\Lambda_I^\hbar(k) \cap \Lambda_1^\hbar(k)$ and $n := \mathcal{I}_k(\ell^*)$ and the identity

$$\bar{v}(x) = \partial_P K(P) \qquad (P \in \mathcal{J}^\infty, x \in T(\{P\} \times \mathbb{T}))$$

for the group velocity on the KAM tori which we both prove now.

By definition (18) of $\mathcal{F}\Lambda_I^\hbar(k)$, the eigenvalue $E_n^\hbar(k)$ is non-degenerate so that

$$\bar{v}_n^\hbar(k) = \left\langle \psi_n^\hbar(k), \bar{v}^\hbar(k)\psi_n^\hbar(k)\right\rangle \tag{31}$$

For ϕ in the (k–invariant) domain of $H^\hbar(k)$ and $E \in \mathbb{R}$ we have the estimate

$$\frac{1}{2}\|\bar{v}^\hbar(k)\phi\|^2 \leq \|(H^\hbar(k) - E)\phi\|\|\phi\| + \|V - E\|\|\phi\|^2 \qquad (k \in \mathbb{T}^*).$$

It follows from Theorem (4.1) that

$$\|\bar{v}^\hbar(k)(\psi^\hbar_{\mathcal{I}_k(\ell^*)}(k) - \tilde{\psi}^\hbar_{\ell^*}(k))\| = \mathcal{O}\left(\hbar^N\right)$$

which implies for the expectation

$$\bar{v}_n^\hbar(k) = \left\langle \psi_n^\hbar(k), (D + \hbar k)\psi_n^\hbar(k)\right\rangle = \left\langle \tilde{\psi}^\hbar_{\ell^*}(k), (D + \hbar k)\tilde{\psi}^\hbar_{\ell^*}(k)\right\rangle + \mathcal{O}\left(\hbar^N\right). \tag{32}$$

By construction of the quasimodes

$$\left\langle \tilde{\psi}^\hbar_{\ell^*}(k), (D + \hbar k)\tilde{\psi}^\hbar_{\ell^*}(k)\right\rangle = \int_{\mathbb{T}} \partial_q \tilde{S}(P, q)\ d\mu_P(q) + \mathcal{O}(\hbar) \tag{33}$$

for $P := \hbar(\ell^* + k), \tilde{S}$ as defined in (14), and

$$d\mu_P(q) := \frac{\partial^2_{qP}\tilde{S}(P, q)\ dq}{\int_{\mathbb{T}} \partial^2_{q'P}\tilde{S}(P, q')\ dq'}.$$

Finally from the Hamilton–Jacobi equation, since the classical flow is ergodic on the invariant torus indexed by P, and since $d\mu_P$ is the invariant measure in q coordinates, it holds

$$\bar{v}(x) = \int_{\mathbb{T}} \partial_q \tilde{S}(P, q)\ d\mu_P(q) = \partial_P K(P) \qquad (P \in \mathcal{J}^\infty, x \in T(\{P\} \times \mathbb{T})).$$

Thus (30) follows from (31), (32) and (33). $\square$

Remark 5.4 Actually we have proven in addition to Theorem 3.1 that $\tilde{\psi}^\hbar_{\ell^*}(k)$ lead to joint quasimodes of $H^\hbar(k), \bar{v}^\hbar(k)$, namely:

$$\|(\bar{v}^\hbar - \partial_P K(\hbar(\ell^* + k)))\tilde{\psi}^\hbar_{\ell^*}(k)\| = \mathcal{O}(\hbar) \qquad (k \in \mathbb{T}^*, \ell^* \in \mathcal{F}\Lambda_I^\hbar(k)).$$

6 Beyond KAM

Theorem 5.3 gives a partial answer to Conjecture 5.1, based on the KAM region $\mathcal{K}_I \subset \mathcal{P}_I$. But what happens in the complement $\mathcal{K}_I^c$? There the classical dynamics is very complicated in general, since one may encounter there further KAM tori (not predicted by the estimates), Cantori, elliptic and hyperbolic periodic orbits, large ergodic components etc.

With the exception of the elliptic orbits, there is no direct generalization of the above KAM methods, and thus it seems hopeless to control the wavefunctions semiclassically supported in that region. However, as the following example shows, other methods may work.

Example. Consider $d = 2$ dimensions. As shown in [2], in the presence of at least two geometrically distinct KAM tori the motion on Σ_E is ballistic ($\bar{v} \neq 0$). This is caused by the fact that these tori have codimension one in Σ_E and thus confine the flow between them. We denote by $\mathcal{R}_I \subset \mathcal{P}_I$ the phase space region enclosed by two nearby KAM tori (or rather families of such tori indexed by the energy in I).

Using microlocal techniques, Shnirelman showed in [8] the existence of a large number of quasimodes concentrated in $\mathcal{R}_I$, see also [3]. Now for large energy E the variation of $\bar{v}$ w.r.t. the restriction of Liouville measure to $\mathcal{R}_I$ is small in comparison with E. Thus by Egorov's Theorem the above quasimodes have group velocities near the classical $\bar{v}$ values (see also [2], Sect. 5).

Different such regions $\mathcal{R}_I$, however, have different classical asymptotic velocities. Thus one should be able to apply the heuristics developed in Sect. 2 to that case, too — *without explicitly knowing the quasimodes*.

When trying to work on this kind of arguments, one is led to the paradoxical conclusion that sometimes it is more useful to know quasimodes (with certain additional properties) of an operator than to know its eigenfunctions.

To explain this, consider the algebra generated by

$$\{H^\hbar(k), \bar{v}_1^\hbar(k), \ldots, \bar{v}_d^\hbar(k)\},$$

$\bar{v}_i^\hbar$ being the components of the operator of asymptotic velocity – which commute with $H^\hbar(k)$ – and try to show the existence of *joint* quasimodes. Arguing along the lines of Sect. 2, such an existence proof could suffice to prove Conjecture 5.1 in full generality.

References

[1] Arnold, V.I.: *Modes and quasi-modes.* Funct. Anal. and its Appl. **5**, 94–101, (1972)

[2] Asch, J., Knauf, A.: *Motion in Periodic Potentials.* Nonlinearity **11**, 175–200 (1998)

[3] Colin de Verdière, Y.: KAM et limites semi-classiques. Dijon, 17-19 septembre 1997, Workshop on KAM in Quantum Mechanics.

[4] Dobrokhotov, S., Shafarevich, A.: *'Momentum' tunneling between tori and the splitting of eigenvalues of the Beltrami-Laplace operator on Liouville surfaces.* Institute for Problems in Mechanics Preprint **599** (1997)

[5] Knauf, A.: *Coulombic Periodic Potentials: The Quantum Case.* Annals of Physics **191**, 205–240 (1989)

[6] Lazutkin, V. F.: *KAM theory and semiclassical approximations to eigenfunctions.* Ergebnisse der Mathematik und ihrer Grenzgebiete, Vol. **24**. Berlin; New York: Springer 1993.

[7] Pöschel, J.: *Integrability of Hamiltonian systems on Cantor sets.* Commun. Pure Appl. Math. **35**, 653–696 (1982)

[8] Shnirelman, A.I.: *On the Asymptotic Properties of Eigenfunctions in the Region of Chaotic Motion.* Addendum to [6]

[9] Reed, M., Simon, B.: *Methods in Mathematical Physics, Vol. IV: Analysis of Operators.* New York: Academic Press 1978

[10] Thomas, L.E.: *Time dependent approach to Scattering from impurities in a Crystal.* Commun. Math. Phys. **33**, 335–343 (1973)

[11] Thomas, L.E., Wassell, S.R.: *Semiclassical Approximation for Schrödinger Operators at High Energy.* In: *Schrödinger Operators*, Lecture Notes in Physics **403**, ed. E. Balslev. New York: Springer 1992

[12] Weiss, D., Lütjering, G., Richter, K.: *Chaotic Electron Motion in Macroscopic and Mesoscopic Antidot Lattices.* Chaos, Solitons & Fractals **8**, 1337 (1997)

[13] Wilcox, C.H.: *Theory of Bloch waves.* Journ. d' Anal. Math. **33**, 146–167 (1978)